NMR Spectroscopic Approaches to Materials. A Case Study in Batteries and Supercapacitors

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Last year, the Swedish Research Council VR granted a new national infrastructure SwedNMR. Distributed over nine Swedish universities, the network is tasked by facilitating and broadening access to NMR spectroscopy. One of the three access nodes (located jointly at Stockholm University and KTH Royal Institute of Technology) handles applications of NMR to materials while the other nodes concern biomolecular and medical applications such NMR-based metabolomics.

Arguably, NMR in materials is an extremely heterogeneous area and, perhaps by tradition, material scientists are not the most ardent users of this methodology. In this lecture we wish to highlight the ways the rich variety of NMR-based experiments can be applied to materials. We shall also illustrate the potential and comparative advantage with NMR that can be realized despite its disadvantages (among other things, its low signal strength and its interpretational pitfalls primarily connected to its tendency to make structural information dependent on the dynamical regime).

Our illustrative examples are going to be taken from the family of materials that, when combined into devices like batteries and supercapacitors, permit us to store electric energy. We shall emphasize that in battery and supercapacitor materials NMR approaches adapted to either the electrodes or the electrolyte can provide direct and local structural and dynamical information about the most crucial component in those systems: the ions. As we are also going to show, a lot what can be learned from NMR is not accessible by other methods. In an orthogonal manner, we shall also try to illustrate what possible insights can be gained from different sorts of NMR parameters like chemical shifts and line splittings (chemical/electronic environments and mesoscopic structures), spin relaxation times (local dynamics), self-diffusion and electrokinetic coefficients (long range dynamics of molecules and ions) and, on a distinct manner, by NMR (or, MRI) images.